### Exceptional service in the national interest



# The *Peridigm* Framework for Peridynamic Simulations

12<sup>th</sup> U.S. National Congress on Computational Mechanics 22 July 2013

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### Peridigm Contributors



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### Outline



- Brief introduction to peridynamics
- The Peridigm code
  - Software design
  - Current capabilities
  - Extending Peridigm
- Performing an analysis with Peridigm
  - Discretization
  - Input deck
  - Post-processing
- Example analyses and ongoing work
  - Many!

### Peridynamic Theory of Solid Mechanics

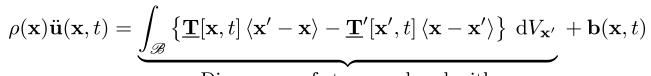


#### WHAT IS PERIDYNAMICS?

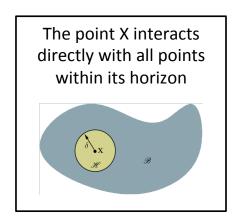
Peridynamics is a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles.

#### **HOW DOES IT WORK?**

- Peridynamics is a nonlocal extension of continuum mechanics
- Remains valid in presence of discontinuities, including cracks
- Balance of linear momentum is based on an integral equation:



Divergence of stress replaced with integral of nonlocal forces.







#### CONSTITUTIVE LAWS IN PERIDYNAMICS

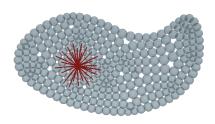
- Peridynamic bonds connect any two material points that interact directly
- Peridynamic forces are determined by force states acting on bonds

$$\underbrace{\mathbf{T}[\mathbf{x},t]}_{\text{Force State}} \underbrace{\langle \mathbf{x}_i' - \mathbf{x} \rangle}_{\text{Bond}}$$

- Force states are constitutive laws that are functions of the deformations of all points within a neighborhood
- Material failure is modeled through the breaking of peridynamic bonds

#### DISCRETIZATION OF A PERIDYNAMIC BODY

 A body may be represented by a finite number of particles (sphere elements) <sup>1</sup>



$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x},t) = \sum_{i=0}^{N} \left\{ \underline{\mathbf{T}}[\mathbf{x},t] \left\langle \mathbf{x}_i' - \mathbf{x} \right\rangle - \underline{\mathbf{T}}'[\mathbf{x}_i',t] \left\langle \mathbf{x} - \mathbf{x}_i' \right\rangle \right\} \Delta V_{\mathbf{x}_i'} + \mathbf{b}(\mathbf{x},t)$$

### Constitutive Models for Peridynamics



#### PERIDYNAMIC FORCE STATES MAP BONDS TO PAIRWISE FORCE DENSITIES

- Peridynamic constitutive laws can be grouped into two categories
  - Bond-based: bond forces depend only on a single pair of material points
  - State-based: bond forces depend on deformations of all neighboring material points

#### Microelastic Material <sup>1</sup>

- Bond-based constitutive model
- Pairwise forces are a function of bond stretch

$$s = \frac{y - x}{x}$$

 Magnitude of pairwise force density given by

$$\underline{t} = \frac{18k}{\pi \delta^4} \varepsilon$$

### <u>Linear Peridynamic Solid</u> <sup>2</sup>

- State-based constitutive model
- Deformation decomposed into deviatoric and dilatational components

$$\theta = \frac{3}{m} \int_{\mathcal{H}} (\underline{\omega} \, \underline{x}) \cdot \underline{e} \, dV \qquad \underline{e}^d = \underline{e} - \frac{\theta \, \underline{x}}{3}$$

Magnitude of pairwise force density given by

$$\underline{t} = \frac{3k\theta}{m} \,\underline{\omega} \,\underline{\mathbf{x}} + \frac{15\mu}{m} \,\underline{\omega} \,\underline{e}^{\mathbf{d}}$$

#### **Definitions**

<u>x</u>	bond vector
x	initial bond length
y	deformed bond length
s	bond stretch
$\underline{e}$	bond extension
$\underline{e}^d$	deviatoric bond extension
$\underline{\omega}$	influence function
V	volume
$\mathcal{H}$	neighborhod
m	weighted volume
$\theta$	dilatation
$\delta$	horizon
k	bulk modulus
$\mu$	shear modulus
$\underline{t}$	pairwise force density

- 1. S.A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48:175-209, 2000.
- 2. S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.

### Classical Material Models Can Be Applied in Peridynamics



#### CORRESPONDENCE APPROACH RESULTS IN A NON-ORDINARY STATE-BASED MATERIAL MODEL 1

 Approximate deformation gradient based on initial and current locations of material points in family

### Approximate Deformation Gradient

### $egin{array}{ccc} \mathbf{X} & ext{reference position} \ \mathbf{X} & ext{vector state} \end{array}$

 $\bar{\mathbf{F}} = (\underline{\mathbf{Y}} * \underline{\mathbf{X}}) \, \mathbf{K}^{-1}$ 

- $\mathbf{K} = \underline{\mathbf{X}} * \underline{\mathbf{X}}$
- Kinematic data passed to classical material model
- Classical material model computes stress
- Stress converted to pairwise force density

$$\underline{\mathbf{T}}\langle \xi \rangle = \underline{\omega} \langle \xi \rangle \ \sigma \mathbf{K}^{-1} \xi$$

- Suppression of zero-energy modes (optional) <sup>2</sup>
- 1. S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.
- 2. Littlewood, D. A Nonlocal Approach to Modeling Crack Nucleation in AA 7075-T651. Proceedings of the ASME 2011 International Mechanical Engineering Congress and Exposition, Denver, Colorado, 2011.

Definitions





#### PERIDYNAMIC OPERATORS ARE ANALOGUES OF THE CLASSICAL THEORY

Relation	Peridynamic Theory	Standard Theory
Kinematics	$\underline{\mathbf{Y}}\langle \mathbf{x}' - \mathbf{x} \rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$	$\mathbf{F} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear Momentum Balance	$\rho\ddot{\mathbf{u}}(\mathbf{x}) = \int_{\mathcal{H}_{\mathbf{x}}} \left\{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle \right\} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x})$	$\rho \ddot{\mathbf{u}}(\mathbf{x}) = \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive Model	$\underline{\mathbf{T}} = \widehat{\mathbf{T}}(\underline{\mathbf{Y}})$	$oldsymbol{\sigma} = \widehat{oldsymbol{\sigma}}(\mathbf{F})$
Angular Momentum Balance	$\int_{\mathcal{H}_{\mathbf{x}}} \left\{ \underline{\mathbf{Y}} \left\langle \mathbf{x}' - \mathbf{x} \right\rangle \times \underline{\mathbf{T}} \left\langle \mathbf{x}' - \mathbf{x} \right\rangle \right\} dV_{\mathbf{x}'} = 0$	$oldsymbol{\sigma} = oldsymbol{\sigma}^T$





#### THE CRITICAL-STRETCH MODEL IS THE SIMPLEST BOND-FAILURE LAW 1

- A bonds fails when its extension exceeds a critical value
- Bond failure is irreversible

$$s_{\max} = \frac{\|\underline{e}\|_{\max}}{\|\underline{x}\|}$$

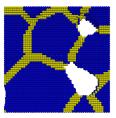
$$\phi = \begin{cases} 0 & \text{if} \quad s_{\text{max}} < s_{\text{crit}} \\ 1 & \text{if} \quad s_{\text{max}} \ge s_{\text{crit}} \end{cases}$$

- Damage results from the accumulation of broken bonds
- Critical stretch parameter is tied to the energy release rate (experimentally measureable)

# *Example*: Modified critical-stretch law for polycrystalline materials <sup>2</sup>

 Modified critical-stretch law for failure of polycrystalline material





- Bond failure law favors material damage along grain boundaries
- Contact algorithm controls material interactions after bonds are broken

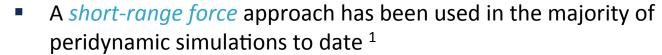
<sup>1.</sup> Silling, S.A. and Askari, E. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures* 83:1526-1535, 2005.

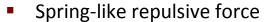
<sup>2.</sup> D. Littlewood, V. Tikare, and J. Bignell. Informing Macroscale Constitutive Laws through Modeling of Grain-Scale Mechanisms in Plutonium Oxide. Workshop on Nonlocal Damage and Failure: Peridynamics and Other Nonlocal Models, San Antonio, Texas, March 11-12 2013.

### **Contact in Peridynamic Simulations**



- Contact algorithms involve two distinct steps
  - Proximity search
  - Enforcement of the contact model



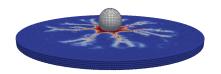


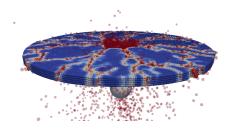
Active when relative distance, r, is below contact radius, r<sub>c</sub>

$$f_{c} = \begin{cases} C(r_{c} - r) \Delta V_{1} \Delta V_{2} & \text{if } r \leq r_{c} \\ 0 & \text{if } r > r_{c} \end{cases}$$

- Does not require explicit definition of contact surfaces
- Friction may be incorporated by decomposing relative motion into normal and tangential components
- More sophisticated contact models are possible
  - Example: iterative penalty enforcement to drive the contact gap to zero <sup>2</sup>







Simulation of brittle fracture

<sup>1.</sup> Silling, S.A. and Askari, E. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures* 83:1526-1535, 2005.

<sup>2.</sup> SIERRA Solid Mechanics Team, Sierra/SolidMechanics 4.22 user's guide, SAND Report 2011-7597, Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2011.

### Outline



- Brief introduction to peridynamics
- The *Peridigm* code
  - Software design
  - Current capabilities
  - Extending Peridigm
- Performing an analysis with *Peridigm* 
  - Discretization
  - Input deck
  - Post-processing
- Example analyses and ongoing work

### The *Peridigm* Computational Peridynamics Code



#### WHAT IS PERIDIGM?

- Open-source software developed at Sandia National Laboratories
- C++ code based on Sandia's Trilinos project
- Platform for multi-physics peridynamic simulations
- Capabilities:
  - State-based constitutive models
  - Implicit and explicit time integration
  - Contact for transient dynamics
  - Large-scale parallel simulations
- Compatible with pre- and post-processing tools
  - Cubit mesh generation
  - Paraview visualization tools
  - SEACAS utilities
- Designed for extensibility





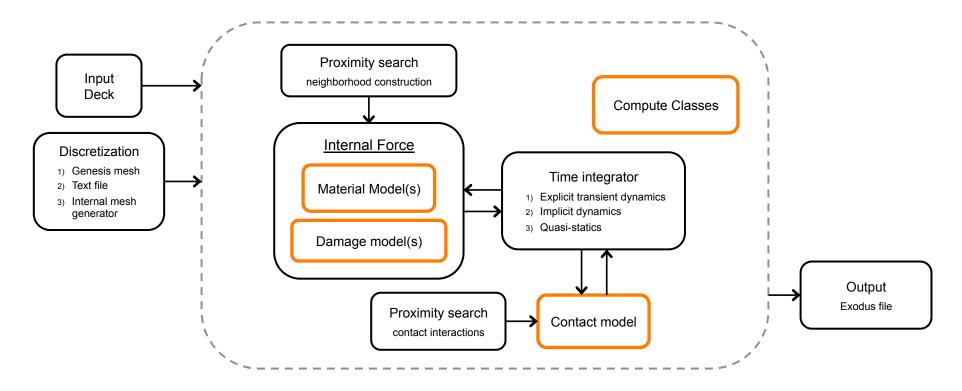
### Peridigm Code Architecture



#### **DESIGN GOALS:**

- State-based peridynamics
- Explicit and Implicit time integration
- Contact

- Performance
- Massively parallel
- Extensibility



Orange denotes extensible components

### Time Integration



#### AVAILABLE INTEGRATION SCHEMES

- Explicit dynamics: Velocity-Verlet (leapfrog) time integrator
- Implicit dynamics: Newmark-beta
- Quasi-statics: Nonlinear solver with modified Newton approach

#### LINEAR SOLVERS

- Iterative Krylov methods, parallel scalability
- Conjugate gradient solver (default solver)
- Wide variety of options available through the Trilinos NOX package

#### CONSTRUCTION OF THE TANGENT MATRIX

- Three options for construction of the tangent matrix:
  - User-supplied tangent
  - Finite-difference scheme
  - Automatic differentiation via the Trilinos Sacado package
- Finite-difference scheme operates directly on internal-force calculation
  - No additional development required by material model developer
- Automatic differentiation approach requires C++ templates and (minor) extension of material model

### Available in Peridigm as of July 2013



#### MATERIAL MODELS

- Linear peridynamic solid <sup>1</sup>
- Elastic-perfectly-plastic <sup>2</sup>

#### DAMAGE MODELS

Critical stretch 5

#### CONTACT MODELS

Short-range force model 5

#### COMPUTE CLASSES

- Output of any node or element variable
- Per-block quantities (min, max, sum)
- Energy (kinetic, stored elastic)

- Elastic-plastic with isotropic hardening <sup>3</sup>
- Viscoelastic <sup>4</sup>
- Thermoelastic (thermal strains)

Neighborhood statistics (horizon, number of neighbors)

Short-range force model with friction

- Approximate deformation gradient <sup>1</sup>
- Many others...
- 1. S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.
- 2. J.A. Mitchell. A nonlocal, ordinary, state-based plasticity model for peridynamics. Sandia Report SAND2011-3166, 2011.
- 3. J.T. Foster, D.J. Littlewood, J.A. Mitchell, and M.L. Parks. Implicit-time integration of an ordinary state-based peridynamic plasticity model with isotropic hardening. ASME International Mechanical Engineering Congress and Exposition, Houston, Texas, November 9-15, 2012.
- 4. J.A. Mitchell. A non-local, ordinary-state-based viscoelasticity model for peridynamics, Sandia Report SAND2011-8064, 2011.
- 5. Silling, S.A. and Askari, E. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures* 83:1526-1535, 2005.



### Extending Peridigm: Adding a Material Model

- Peridigm material models derive from the Material base class
- Specify required data fields
- Required routines

Optional routines

Others...

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### Performing an Analysis with Peridigm



#### CREATING A DISCRETIZATION

#### Option 1) Genesis file

- Cubit mesh generator (hexahedron or tetrahedron mesh)
- Designate blocks and node sets
- Genesis sphere meshes also supported

#### Option 2) Text file

- Discretization defined by (coordinates, volume, block id) at each node
- User-supplied node sets (lists of node ids)
- Supports EMU input files

#### Option 3) Internal mesh generator

- Rectangular or cylindrical solid
- Restricted to single block
- User-supplied node sets (lists of node ids)

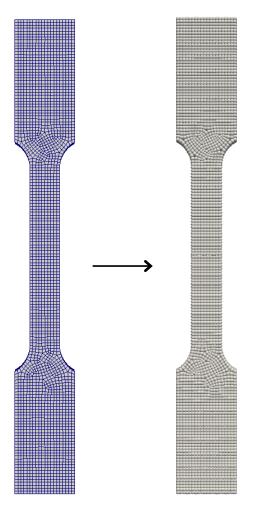


Illustration of *Peridigm* conversion from hexahedron mesh to sphere mesh

### Performing an Analysis with Peridigm



#### CREATING AN INPUT DECK

```
Discretization
    Type "Exodus"
    Input Mesh File "tensile test.g"
Materials
    My Material
      Material Model "Elastic"
      Density 8.0
      Bulk Modulus 1.500e12
      Shear Modulus 6.923e11
Blocks
    My Block
        Block Names "block 1 block 2 block 3"
        Material "My Material"
        Horizon {0.1900*2.1/2.0}
Boundary Conditions
    Prescribed Displacement Bottom
        Type "Prescribed Displacement"
        Node Set "nodelist 1"
        Coordinate "y"
        Value "y*0.01*t"
```





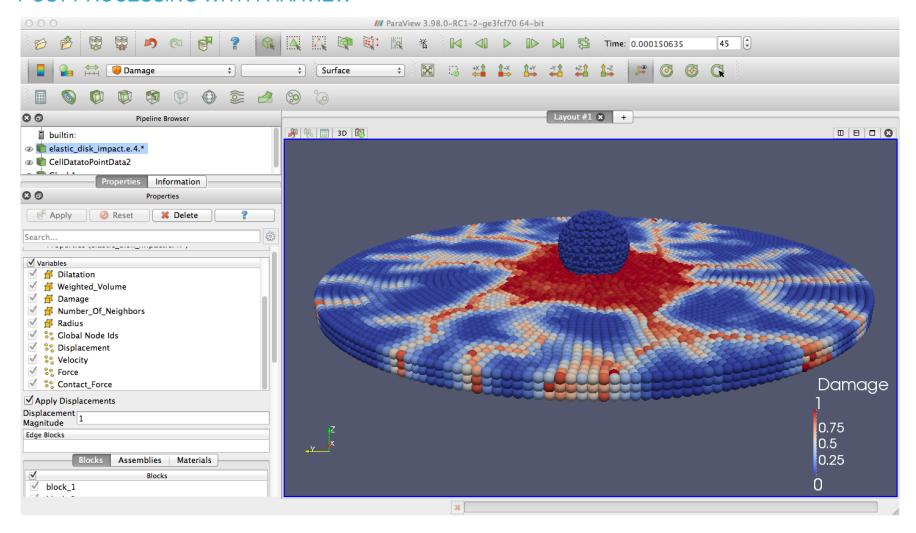
#### CREATING AN INPUT DECK (CONTINUED)

```
Solver
    Initial Time 0.0
   Final Time 1.0
    QuasiStatic
        Number of Load Steps 4
        Absolute Tolerance 1.0
        Maximum Solver Iterations 10
Compute Class Parameters
    Strain Gage Top Displacement
        Compute Class "Nearest Point Data"
        X 0.0
        Y 1.27
        Z 0.0
        Variable "Displacement"
        Output Label "Gage Top Displacement"
Output
    Output File Type "ExodusII"
    Output Filename "tensile test"
    Output Frequency 1
    Output Variables
        Dilatation "true"
        Gage Top Displacement "true"
```

### Performing an Analysis with Peridigm



#### POST-PROCESSING WITH PARAVIEW 1



1. www.paraview.org

### Outline



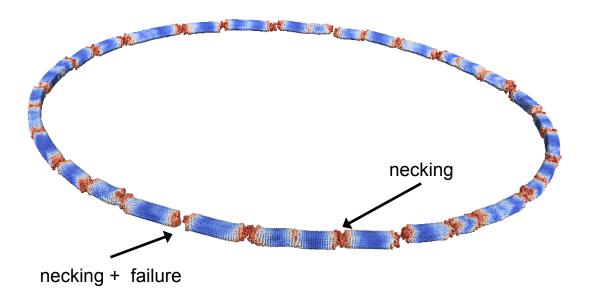
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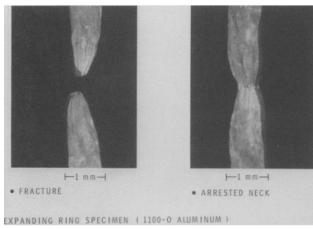
### **Elastic-Plastic Material Model**



#### PERIDIGM PREDICTS NECKING AND FRAGMENTATION OF EXPANDING RING

- Motivated by ring fragmentation experiments of Grady and Benson <sup>1</sup>
  - 1100-0 aluminum ring (ductile)
- Modeled in Peridigm with elastic-perfectly-plastic constitutive model <sup>2</sup>





Fracture and arrested neck region from electromagnetically-loaded expanding ring <sup>1</sup>

- 1. D. Grady and D. Benson. Fragmentation of metal rings by electromagnetic loading, *Experimental Mechanics*, 23(4), 1983.
- 2. J.A. Mitchell. A nonlocal, ordinary, state-based plasticity model for peridynamics. Sandia Report SAND2011-3166, 2011.

### Thermoelastic Material Model



#### MODIFY BOND EXTENSION TO INCORPORATE THERMAL EXPANSION / CONTRACTION

#### Thermoelastic Linear Peridynamic Solid

 Linear relationship between temperature change and thermal bond extension

$$\underline{e}^{\text{thermal}} = \alpha \, \Delta T \, \underline{x}$$

where  $\alpha$  is the thermal expansion coefficient

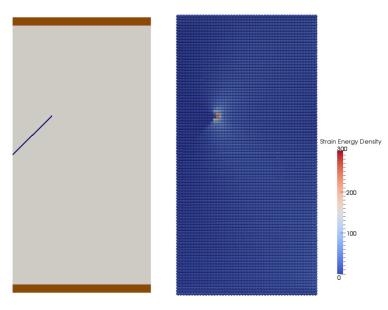
Subtract thermal extension from total extension

$$\underline{e}^* = \underline{e} - \underline{e}^{\text{thermal}} = \underline{e} - \alpha \, \Delta T \, \underline{x}$$
$$\theta^* = \int_{\mathcal{H}} \frac{3}{m} \, (\underline{\omega} \, \underline{x}) \cdot \underline{e}^* \, dV$$

$$\underline{e}^{*d} = \underline{e}^* - \frac{\theta^* \, \underline{x}}{3}$$

$$\underline{t}^* = \frac{3k\theta^*}{m}\underline{\omega}\underline{x} + \frac{15\mu}{m}\underline{\omega}\underline{e}^{*d}$$

#### Pre-cracked plate under thermal load



- Fixed displacement at ends of plate
- Uniform temperature reduction
- Strain energy concentration results at crack tip

### **Drucker-Prager Plasticity Model**



#### PRESSURE-DEPENDENT YIELD CONDITION APPLICIABLE TO CONCRETE & SOIL

- Ongoing research on nonlocal analog of linear Druker-Prager plasticity model
  - Pressure-dependent peridynamic yield criterion and flow rule
  - Motivated by pressure-dependent material response over multiple length scales
  - Dissipation-governed bond failure law also under development

Goal: Analyze multiscale, dynamic failure of concrete during impact

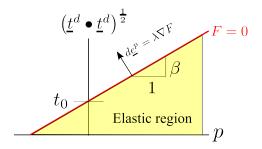
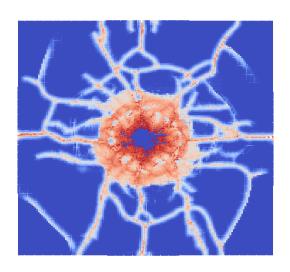


Illustration of plastic flow rule



Simulated concrete impact

[Christopher Lammi]



#### Sandia National Laboratorie

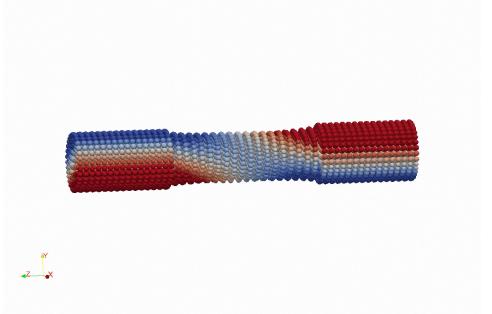
### Quasi-static Preload for Transient Dynamics Simulation

#### SINGLE SIMULATION ENCORPORATING MULTIPLE TIME INTEGRATION SCHEMES

Employ multiple solvers

```
Solver1
Initial Time 0.0
Final Time 0.6
QuasiStatic
Number of Load Steps 6
Absolute Tolerance 1.0
Maximum Solver Iterations 100

Solver2
Initial Time 0.6
Final Time 0.601
Verlet
Fixed dt 1.5e-7
```



Utilize ternary operator in definition of boundary conditions

```
Boundary Conditions
Prescribed Displacement Bottom x
   Type "Prescribed Displacement"
   Node Set "nodelist_1"
   Coordinate "x"
   Value "t <= 0.6 ? x*cos(1.5*t)-y*sin(1.5*t) : x*cos(1.5*0.6)-y*sin(1.5*0.6)"</pre>
```

[John Foster]

### **Surface Correction Factor**



#### **CHALLENGE**

- The majority of peridynamic material models were derived based on bulk response
- Material points close to the surface have reduced nonlocal region (fewer bonds) than material points in the bulk
- Ordinary peridynamic material models exhibit inconsistencies at the surface

#### POTENTIAL SOLUTION

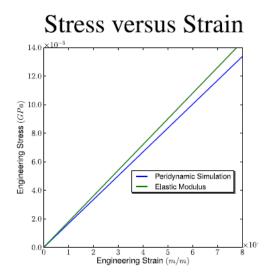
Modify material model near surfaces to mitigate surface effect

### **Axial Displacement**



#### **Sources of Error**

- Geometric surface effects
- Nonlocal model (dilatation on surface) and related model properties
- 3) Discretization error



[John Mitchell]

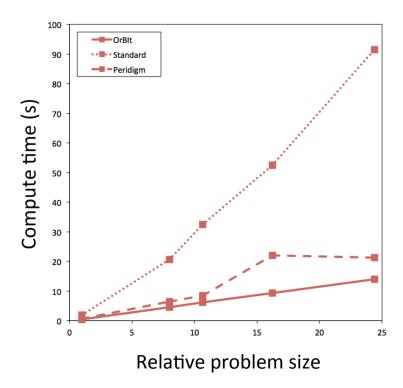
### Matrix Assembly via Bond Iteration



#### NOVEL MATRIX ASSEMBLY SCHEME REDUCES COST OF IMPLICIT ANALYSES

- Ongoing algorithmic research on assembly of nonlocal tangent stiffness matrix
- Initial results show 3-4 x speedup in assembly time over cell iteration
- Broken bonds can be removed from iteration loop
- Computes sensitivities for a single row simultaneously (saves on sparse matrix insertion)
- Simplified control of damage propagation in quasi-static analyses
- Applicable to current *Peridigm* code architecture

#### Comparison of serial assembly time

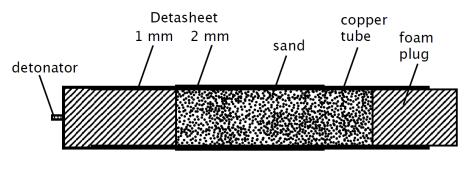


### **Explosively Compressed Cylinder**



#### PERIDYNAMICS ENABLES MODELING OF PERVASIVE MATERIAL DAMAGE

- Motivated by experiments of Vogler and Lappo <sup>1</sup>
- Commonly used approach for consolidation of powders
- Copper cylinder filled with granular material and wrapped with Detasheet explosive
- Polyurethane foam plugs used to keep granular sample in tube





Cylinder schematic

Cylinder after compression

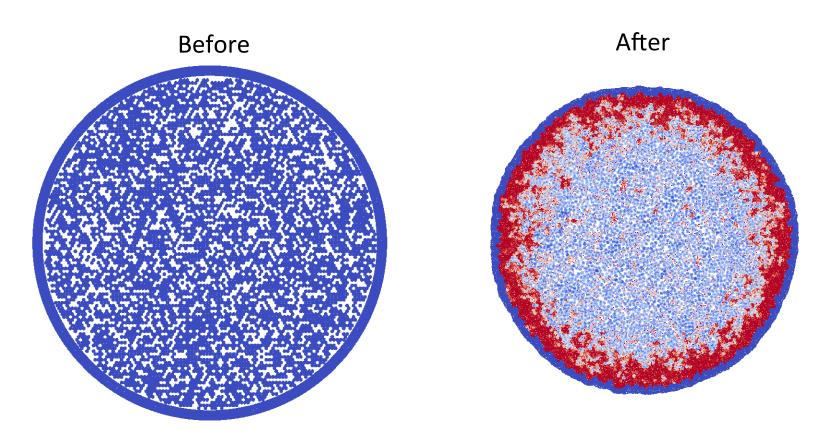
### [Tracy Vogler]

1. T.J. Vogler and K.M. Lappo. Cylindrical compaction of granular ceramics: experiments and simulations, The 12<sup>th</sup> Hypervelocity Impact Symposium, 2012.

### **Explosively Compressed Cylinder**



#### COMPUTATIONAL RESULTS OBTAINED WITH PERIDIGM



Color denotes damage (percentage of broken bonds)

[Tracy Vogler, John Foster, Canio Hoffarth]

# Improved Digital Image Correlation (DIC) using Peridynamic Damage Modeling



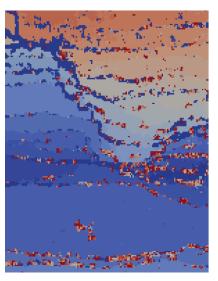
#### CHALLENGE

- DIC often fails near cracks or discontinuities
- Displacements obtained by interpolation across a crack are highly inaccurate

#### POTENTIAL SOLUTION

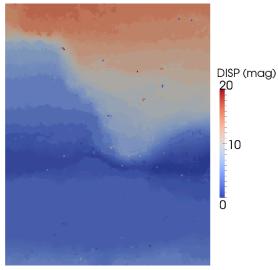
- Apply peridynamics to compute displacements in regions where DIC fails
- Treat the quality DIC displacements as boundary condition and solve for the remainder of the domain using a peridynamic model

# Failure of fiber-reinforced concrete tensile specimen



Dark blue regions denote failed correlation, spurious colors represent inaccurate displacements

Standard DIC



Enhanced result

Peridynamic approach
improves correlation

[Daniel Turner]

### Application of Peridynamics to Digital Image



#### INITIAL RESULTS

- Computed damage profile closely matches experimental results
- Displacement (strain) accuracy is considerably improved

### Failure of fiber-reinforced concrete tensile specimen

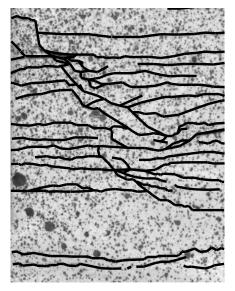
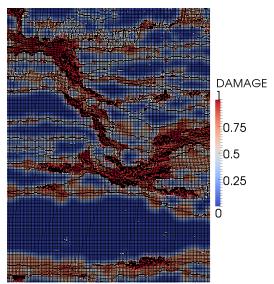


Photo of damaged concrete specimen

Peridynamic damage profile Lines indicate cracks



### Ongoing and Future Work



- Coupling to local models
  - Work underway to couple Peridigm with the classical FEM code Albany
- Expanded contact functionality
  - User-defined block-by-block contact interactions
  - Improved parallel proximity search
- Advanced control over bond initialization
  - Allow for bond cutting with mesh entities (e.g., shell elements) <sup>1</sup>
- Bond failure in quasi-static simulations
  - Requires iterative solution of model problems

<sup>1.</sup> SIERRA Solid Mechanics Team, Sierra/SolidMechanics 4.22 user's guide, SAND Report 2011-7597, Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2011.

### Questions?



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